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# The role of multiple electron capture in the x-ray emission process following charge exchange collisions with neutral targets

S. Otranto<sup>1</sup>, N. D. Cariatore<sup>1</sup> and R. E. Olson<sup>2</sup>

<sup>1</sup>IFISUR and Departamento de Física, Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina.

<sup>2</sup>Physics Department, Missouri University of Science and Technology, Rolla MO 65409, USA.

sotranto@uns.edu.ar

**Abstract.** In this work we theoretically study photonic spectra that follow charge exchange processes between highly charged ions and neutral argon and CO targets. The range of collision energies studied is 5 eV/amu-10 keV/amu, covering typical EBIT-traps and Solar Wind energies. Our studies are based on multiple electrons schemes within the classical trajectory Monte Carlo method. Electrons are sorted with the sequential binding energies for the target under consideration. The role played by the multiple electron capture process for the different collision systems under consideration is explicitly analyzed and its contribution separated as arising from double radiative decay and autoionizing multiple capture. Present studies are stimulated by the upcoming launch of the Astro-H mission in 2015, which will provide high resolution spectra in the 0.3 keV-12keV band.

## 1. Introduction

The study of photonic spectra following charge exchange collisions has been a field with growing interest during the past 15 years. The unexpected detection of the X-ray emission from comet P/Hyakutake by ROSAT in 1996 [1], later on ascribed to the charge exchange mechanism between the Solar Wind ions and the neutrals targets in gas phase in the cometary coma [2], triggered a deep search of cometary x-ray sources in other astrophysical environments like planetary atmospheres, the heliosphere, the interstellar medium and even other galaxies. As recently pointed out by Dennerl [3], it seems now strange that such emission had remained unnoticed to us and had been detected even with surprise by the astrophysical community, provided that all the elements to predict such an emission were already at hand by 1968.

By the year 2000, and with the Chandra X-ray Observatory (CXO) already in orbit providing cometary spectra with a much improved resolution of about 100 eV, several laboratories worldwide worked upon the study of the collision processes and the possible recreation of cometary spectra based on laboratory data [4-7]. EBIT traps married to calorimeter spectrometers provided *in-situ* spectra with



an unprecedented resolution of about 8 eV at collision energies which are two orders of magnitude below those corresponding to the Solar Wind. Linear accelerators, on the other hand, reached Solar Wind velocities but missed the dominant forbidden lines  $2^3S \rightarrow 1^1S$  which are long lived and cannot take place within the typical dimensions of the devices under use. Since then, a limited but nonetheless important set of data has been collected by several experimental groups [8].

Theoretical studies in this context, on the other hand, have been mainly conducted by means of the classical overbarrier model [5], the Landau-Zener multichannel model [9] and the classical trajectory Monte Carlo (CTMC) method [10-15]. In addition, electron capture cross sections for hydrogen targets obtained by means of atomic orbitals close coupling codes have been used by Bodewits and Hoekstra to simulate cometary spectra [7] and line emission studies have been also recently made within the two center-basis generator model [16].

A significant problem in this context is that of multiple-electron capture by highly charged ions colliding with multielectronic targets. As multiple capture probabilities are expected to increase with the projectile charge, a key point during the analysis of laboratory and astrophysical spectra is the accurate determination of the fraction of X-rays which originate in multiple electron transfer [13].

In this work, we explicitly evaluate the role of the multiple electron capture process in the photonic spectra which follow charge exchange collisions involving highly charged ions and argon and CO targets. The former target has been largely explored at different laboratories [8,17,18], while the latter is a significant component in cometary environments and can be also found in the atmospheres of Venus and Mars. In section 2, we describe the CTMC models used for the different targets under consideration and the scheme used to account for the Auger cascading processes which ultimately lead to single or double radiative decay. In section 3, we show our main results. Conclusions and outlook are drawn in Section 4.

## 2. Theoretical Method

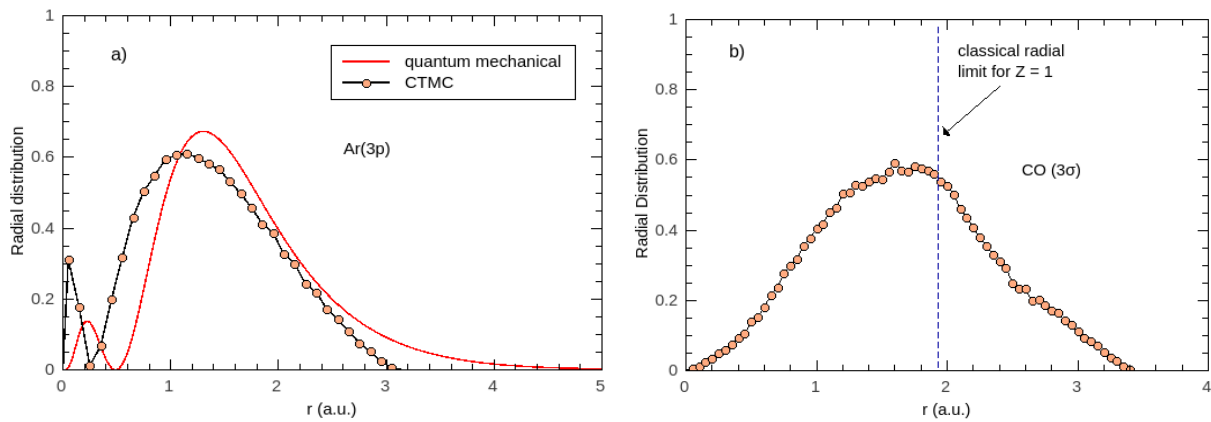
Theoretical electron capture and line emission cross sections have been calculated using the CTMC method [19]. In the following we detail how this method has been adapted for the two targets under consideration and the decay scheme used to account for the Auger cascading processes.

### 2.1 Argon

Hamilton's equations are solved for a system composed by the projectile, the ionic core, and eight non-interacting electrons (the whole M shell) which are sorted according to the sequential binding energies for the target. Although electron-electron correlations are not accounted in detail, the energy deposition needed for many electron removal is properly considered. Electrons are sorted according to the quantum mechanical momentum distribution and their interaction with the ionic core is considered to be Coulomb-like with an effective charge that is set in order to provide the best possible agreement with the quantum mechanical radial distribution. To further exemplify, in figure 1a) we show the radial distribution obtained for the electron initialized with the first ionization potential of 15.7 eV. Interesting to notice, the above detailed procedure correctly leads to the nodal structure in the radial distribution.

### 2.2 CO

For CO we consider a many-electron-multicenter approach. Hamilton's equations are solved for a system composed by the projectile, two ionic centers (fixed in space at the equilibrium distance  $R = 2.13$  a.u.), and eight non-interacting electrons again sorted according to their sequential binding energies.



**Figure 1.** CTMC radial distributions for a) Ar(3p) and b) the  $3\sigma$  orbital of CO.

The molecular axis is randomly oriented and the eight electrons interact with the ionic centers via the pseudopotential developed by Gabas et al. [20]:

$$V_{CO^+}(r_{eC}, r_{eO}) = V_C(r_{eC}) + V_O(r_{eO}),$$

$$V_O(r_{eO}) = -\frac{8 - N_O}{r_{eO}} - \frac{N_O}{r_{eO}} (1 + \alpha_O r_{eO}) e^{-2\alpha_O r_{eO}},$$

$$V_C(r_{eC}) = -\frac{6 - N_C}{r_{eC}} - \frac{N_C}{r_{eC}} (1 + \alpha_C r_{eC}) e^{-2\alpha_C r_{eC}}.$$

The corresponding coefficients are  $N_o = 7.609$ ,  $N_c = 5.391$ ,  $\alpha_o = 1.501$  and  $\alpha_c = 0.85$ .

In figure 1b) we show the radial distribution obtained for the  $3\sigma$  orbital (ionization potential of 14.01 eV). Compared to simpler single-center approaches which model the target as an hydrogenic core of  $Z = 1$  with the ionization potential of the target under consideration, the present multicenter treatment leads to a more extended radial distribution and is expected to provide a more accurate description of the target.

### 2.3 Decay scheme for the multiple-electron capture

The Auger decay scheme used in this work is based in the decay scheme developed by Ali et al [21] for collisions involving argon ions with argon atoms and can be summarized as follows:

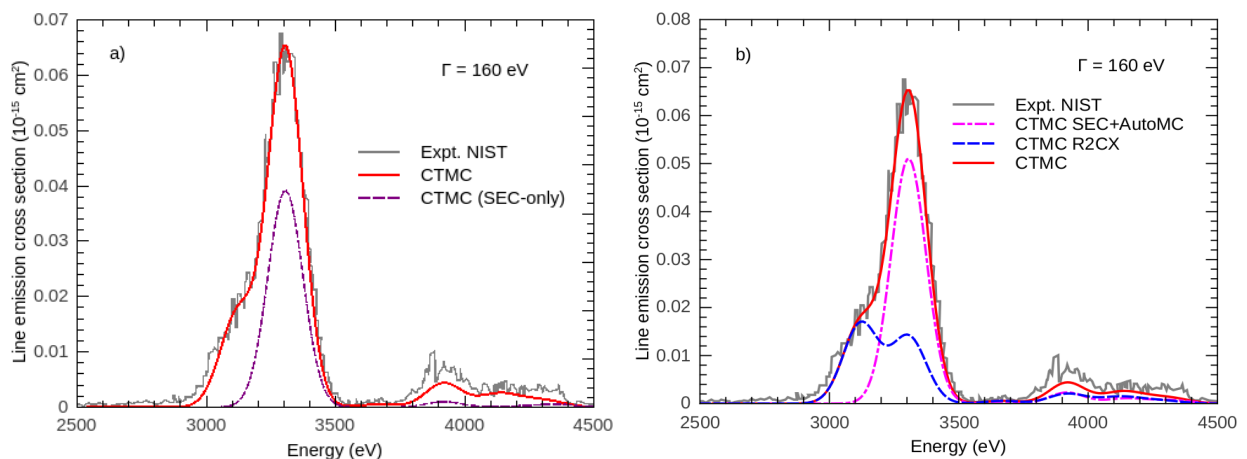
- (i) Multiply excited states dominantly stabilize via multiple Auger processes.
- (ii) Two-electron Auger processes are considered only.
- (iii) Transitions involving electrons in the same shell proceed first. If several electrons are in different shells, the Auger process involves the two electrons which are energetically closer.
- (iv) Each Auger transition proceeds with the unit probability to the nearest continuum limit. The decaying electron falls to a well-established  $n$  level according to the energy equation.

- (v) If the new configuration still provides a multiple excited state involving more than two electrons, those rules are applied again until only two electrons remain bound to the projectile.
- (vi) If a cascading process leads to an asymmetric doubly excited state ( $|n_2 - n_1| \geq 2$ ), the event is characterized as radiative decay (R2CX). Otherwise, a final Auger process takes place and the event is characterized as single charge exchange. As a result, the single charge exchange channel includes the contributions arising from the single electron capture (SEC) and the autoionizing multiple capture (AutoMC) channels.

Finally, we note that the electronic angular momenta of the decaying electrons are determined throughout the Auger process by requiring the preservation of their respective orbital eccentricities. For the sake of simplicity, hydrogenic energy levels are used to determine the projectile population after multiple charge exchange.

### 3. Results

In figure 2 we show the line emission cross sections following  $\text{Ar}^{18+} + \text{Ar}$  charge exchange collisions at an impact energy of 4 keV/amu. Such impact energy is very close to that corresponding to the fast Solar Wind ( $\sim 700$  km/sec). Present theoretical results are compared to the experimental data of Tawara *et al* [8] which are normalized to our theoretical absolute values. Although the reported energy resolution of the detector is roughly 130 eV for Ti Ly- $\alpha$  x-rays at 4.5keV, we convolute our line emission cross sections by means of 160 eV FWHM Gaussian functions in order to match the experimental widths. In figure 2a) we show the separate contribution of the single-electron-capture (SEC) channel. In this case, the fraction of x-rays originating in multiple capture amounts up to 55%.

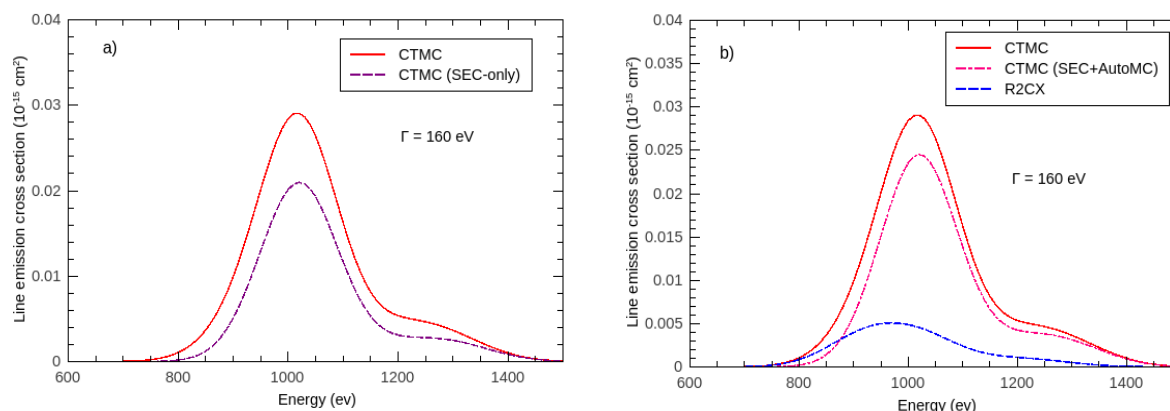


**Figure 2.** CTMC line emission cross sections for 4 keV/amu  $\text{Ar}^{18+} + \text{Ar}$  collisions. Present results are compared to the NIST experimental data of Tawara *et al* [8]. The partial contributions of the SEC channel and the radiative decay (R2CX) are explicitly shown.

In Figure 2b) the autoionizing multiple capture and double radiative decay contributions are individually shown. It can be easily seen that the satellite peak originating in double radiative decay is shifted compared to the hyper-satellite position and provides a low-energy shoulder to the Ly- $\alpha$  peak. Also, the CTMC estimates for the fraction of x-rays due to radiative double decay amount to about

71.4% of the multiple capture channel. Our preliminary results indicate that the fraction of x-rays associated to double radiative decay increases with the projectile charge.

Now moving to the CO target, in figure 3 we show the line emission cross sections following charge exchange reactions in 3.5 keV/amu  $\text{Ne}^{10+} + \text{CO}$  collisions. The impact energy under consideration belongs to the Solar Wind range and has been widely considered by the JPL group during the last decade [4,5]. Present results are again convoluted over an energy resolution of 160 eV FWHM. In this case, the fraction of x-rays originating in multiple capture amounts up to 33%. In figure 3b) the autoionizing multiple capture and double radiative decay contributions are individually shown. The CTMC estimates for the fraction of x-rays due to radiative double decay amount to about 63.5% of the multiple capture channel.



**Figure 3.** CTMC line emission cross sections for 3.5 keV/amu  $\text{Ne}^{10+} + \text{CO}$ . The partial contributions of the SEC channel and the radiative decay (R2CX) are explicitly shown.

In Table 1 we consider the state selective relative populations to  $n = 3$  and 4 in 2.25 keV/amu  $\text{O}^{6+} + \text{CO}$  collisions. The JPL experimental data from Miller *et al* [22] obtained from line emission spectra are shown for comparison. It can be seen that present results are in good agreement with the experiments. Nevertheless, we point out that we have detected a non negligible amount of capture into the 5g state that would entirely feed the 3d + 4f line. For that reason, we have incorporated our 5g state selective cross sections in the results shown.

**Table 1.** State selective relative populations to  $n=3$  and  $n=4$  in 2.25 keV/amu  $\text{O}^{6+} + \text{CO}$  collisions. The experimental data corresponds to Miller *et al* [22].

	Expt	<i>mmCTMC</i>
<b>4p</b>	$0.13 \pm 0.03$	0.169
<b>4d</b>	$0.13 \pm 0.03$	0.121
<b>4s</b>	$0.23 \pm 0.05$	0.174
<b>3p</b>	$0.07 \pm 0.02$	0.089
<b>3d+4f</b>	$0.41 \pm 0.09$	0.360
<b>3s</b>	$0.03 \pm 0.01$	0.085

#### 4. Conclusions

In this work we have theoretically studied the role of the multiple electron capture channel in the x-ray spectra following charge exchange collisions between highly charged ions and neutral targets (argon and CO). A classical trajectory Monte Carlo model based on eight non-interacting electrons sorted with sequential binding energies has been married with a decay scheme which allows the explicit separation of the multiple electron capture events in autoionizing multiple capture (leading to single electron capture) and double radiative emission. Present results for  $\text{Ar}^{18+}+\text{Ar}$  are found in very good agreement with the x-ray spectra of Tawara et al obtained at NIST. Moreover, our calculations nicely reproduce the low energy shoulder in the Ly- $\alpha$  structure which corresponds to the satellite transition and originates in double radiative decay. For  $\text{Ne}^{10+}+\text{CO}$ , on the other hand, our results suggest a not so prominent role for the multiple capture channel. These results indicate that the fraction of x-rays originating in multiple electron capture increases for larger projectile charges. Finally, we contrasted our theoretical results with the relative populations of the  $n = 3$  and 4 levels measured by Miller et al at JPL for 2.25 keV/amu  $\text{O}^{6+}+\text{CO}$  collisions.

New complementary laboratory studies would be welcome at this point to further test our present theoretical capabilities.

#### Acknowledgments

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